HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

C5 Non-Cyclics Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

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PLAIN ENGLISH SUMMARY

This test plan addresses streams which are products of the ethylene process and associated C5 processes and which contain, predominantly, isoprene and/or other C5 or C6 non-cyclic alkenes and alkanes. The plan addresses the category by evaluating four substances: pure isoprene (data are already available except for aquatic toxicity data - an acute algal toxicity study will be conducted), a mid-range isoprene stream containing 14-20 percent isoprene (testing will be conducted), a low concentration stream with approximately 2 percent isoprene (testing will be conducted), and a high-purity 2-methyl-2-butene stream (testing will be conducted). The test plan is based on the expectation that the presence of isoprene and 2-methyl-2-butene will be responsible for the biological activity of the streams. This assumption is based in part on existing data for isoprene and 2-methyl-2-butene, and also on what is known about the other components. Isoprene and 2-methyl-2-butene are sponsored through the ICCA (International Council of Chemical Associations) HPV Program. Additional supporting data will be collected on many of the other components as part of other test plans under the HPV Challenge Program, the ICCA program, or from chemicals already sponsored in the OECD SIDS program.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the test plan for the C5 Non-Cyclics category under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category.

This test plan addresses streams which are products of the ethylene process and associated C5 processes and which contain, predominantly, isoprene and/or other C5 or C6 non-cyclic alkenes and alkanes. The plan addresses the category by evaluating four substances:

- Isoprene

  This is a high purity isoprene stream. Data for HPV endpoints are already available except for aquatic toxicity. An acute algal toxicity study, OECD Guideline 201, will be conducted. In addition, structural activity relationships will be used to predict toxicity to fish and *Daphnia*. Isoprene is sponsored through the ICCA (International Council of Chemical Associations) HPV Program.

- Pyrolysis C5s

  This is a mid-range isoprene stream containing 14-20 percent isoprene. The following studies will be conducted: An Ames test (OECD Guideline 471), a mouse inhalation micronucleus test (OECD Guideline 474), a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422), an algal toxicity test (OECD Guideline 201), a *Daphnia* sp. acute toxicity test (OECD Guideline 202), a fish acute toxicity test (OECD Guideline 203), and a biodegradation test (OECD Guideline 301F).

- Hydrotreated C5s

  This is a low isoprene stream containing approximately 2 percent isoprene. The following studies will be conducted: An Ames test (OECD Guideline 471), a mouse inhalation micronucleus test (OECD Guideline 474), a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422), an algal toxicity test (OECD Guideline 201), a *Daphnia* sp. acute toxicity test (OECD Guideline 202), a fish acute toxicity test (OECD Guideline 203), and a biodegradation test (OECD Guideline 301F).

- 2-Methyl-2-Butene

This is a high purity 2-methyl-2-butene stream. Data are already available for genetic toxicity. The following studies will be conducted: A rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422), an algal toxicity test (OECD Guideline 201), a *Daphnia* sp. acute toxicity test (OECD Guideline 202), a fish acute toxicity test (OECD Guideline 203), and a biodegradation test (OECD Guideline 301F). 2-Methyl-2-butene is sponsored through the ICCA HPV Program.

The test plan is based on the expectation that the presence of isoprene and 2-methyl-2-butene will be responsible for the biological activity of the streams. This assumption is based in part on existing data for isoprene and 2-methyl-2-butene, and also on what is known about the other components. Additional supporting data will be collected on many of the other components as part of other test plans under the HPV Challenge Program, the ICCA program, or from chemicals already sponsored in the OECD SIDS program.

Predictive computer models will be used to develop relevant environmental fate and physiocochemical data for substances in the C5 Non-Cyclics category. Environmental fate information will be summarized either through the use of computer models when meaningful projections can be developed or in technical discussions when computer modeling is not applicable. For mixed streams, physicochemical properties will be represented as a range of values according to component composition. These data will be calculated using a computer model cited in an EPA guidance document prepared for the HPV Challenge Program.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

BP Amoco Chemicals
Chevron Phillips Chemical Company
CONDEA Vista Company*
The Dow Chemical Company
E. I. du Pont de Nemours and Company*
Eastman Chemical Company*
Equistar Chemicals, LP
ExxonMobil Chemical Company
Fina Oil and Chemical Company*
Formosa Plastics Corporation, U.S.A.*
The B.F.Goodrich Company*
The Goodyear Tire & Rubber Company
Huntsman Corporation
Koch Industries*
NOVA Chemicals Inc.
Shell Chemical Company
Sunoco, Inc.*
Texas Petrochemicals Corporation*
Union Carbide Corporation*
Westlake Chemical Corporation*
Williams Olefins, LLC*

* These companies are part of the Olefins Panel but do not produce streams in the C5 Non-Cyclics Category.

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TEST PLAN FOR THE C5 NON-CYCLICS CATEGORY

I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the C5 Non-Cyclics category under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program (Program).

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for substances included in the category, and outlines testing needed to develop screening level data for this category under the Program. This document also provides the testing rationale for the C5 Non-Cyclics category. The objective of this effort is to identify and develop sufficient test data and/or other information to adequately characterize the human and environmental health and environmental fate for the category in compliance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in EPA guidance documents.

II. DESCRIPTION FOR THE C5 NON-CYCLICS CATEGORY

A. The Category

The C5 Non-Cyclics category was developed by grouping ethylene manufacturing streams that the Panel believes are similar from both a process and a toxicology perspective, which is why this group is considered a category for purposes of the HPV Program. Sixteen CAS numbers (Table 1) are used to describe these eleven process streams arising from the ethylene process and other associated C5 processes. Nine of these process streams are complex reaction products. The CAS numbers used to represent these nine products are generally vague with respect to the specifics that distinguish the streams within the category. Therefore a single stream is correctly represented by more than one CAS number and a CAS number may be applicable to more than one stream. A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. A description of the ethylene and associated processes is included in Appendix I.

The streams in this category consist of high purity hydrocarbons and complex hydrocarbon reaction products that contain significant levels of olefins with a carbon number distribution that is predominantly C5 or C6. The typical compositions of the streams are shown in Table 2. All but three of these streams contain isoprene. The three streams that do not contain isoprene consist of C5 and/or C6 alkenes that

are predicted to have a toxicology profile similar to that of the 2% isoprene stream. Typically, only six of the many components of the streams (isopentane, isoprene, pentane, 2-methyl-2-butene, neohexene, 1,3-pentadiene) are present at concentrations ≥30%; and only six more components (2-butene, isopentene, 2-pentene, cyclopentadiene, cyclopentene, methyl-pentenes-2) are present at ≥20%. The category is designated C5 Non-Cyclics.

The CAS Numbers in the C5 Non-Cyclics category are associated with eleven streams which are commercial products or isolated intermediates:

1. Pyrolysis C5s
2. Hydrotreated C5s
3. Pentenes
4. Piperylene Concentrate
5. Isoprene Concentrate
6. Isoprene-Piperylene Concentrate
7. Isoprene, High Purity
8. Isoprene Purification Byproduct
9. 2-Methyl-2-Butene
10. Metathesis Byproduct
11. Neohexene

Descriptions of the eleven streams associated with the C5 Non-Cyclics category are presented below:

1. Pyrolysis C5s

Pyrolysis C5s (or C5 fraction) consist of a hydrocarbon distillate fraction separated from pyrolysis gasoline (the C5+ portion of the cracked gas in the ethylene process). The carbon number distribution of the product is predominantly C5, but the stream also typically contains relatively low levels of the higher boiling C4 substances (e.g. 1,2-butadiene) as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 0.25% and present in the distillate largely due to azeotropes of benzene with other hydrocarbon species in the complex mixture. The 1,3-butadiene content is typically 1%. The stream contains significant levels of olefins, diolefins and cyclics.

2. Hydrotreated C5s

Hydrotreated C5s result from hydrogenation of Pyrolysis C5s over catalyst. Typically the stream that is charged to the hydrogenation reactor is a broader boiling range stream than the C5 fraction. For example, a full range pyrolysis gasoline may be hydrotreated and the resulting product then fractionated to produce the Hydrotreated C5s as a distillate fraction. The hydrogenation process may be either a one-stage or two-stage process. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to monoolefins. The two-stage process is typically a vapor-phase, more severe hydrogenation that converts monoolefins to paraffins. Typically,

Hydrotreated C5s are subject only to one-stage hydrogenation because the product is intended for use in gasoline where the monoolefins are desired components. Similar to Pyrolysis C5s, Hydrotreated C5s have a carbon number distribution that is predominantly C5, and contain low levels of the higher boiling C4 substances as well as low levels of the more volatile C6 hydrocarbons. Benzene content is typically 1%. Unlike pyrolysis C5s, the diolefin content in Hydrotreated C5s is very low.

3. Pentenes

Pyrolysis C5s are typically fractionated into concentrates of the reactive diolefins: isoprene, piperylene (1,3-pentadiene) and cyclopentadiene (as dimer.) As a first step in producing these concentrates, the lighter boiling fraction of the stream, i.e., the compounds that are more volatile than isoprene, are sometimes removed as a distillate. This distillate is designated as Pentenes or the Pentenes Cut. The stream has a carbon number distribution that is predominantly C4-C5, consisting in part of iso-pentane and the more volatile pentenes such as 1-pentene, with about 1-3% isoprene. The stream typically contains the C4 compounds that were present in the Pyrolysis C5s, including 1,3-butadiene. Alternately, Pentenes can be removed later in processing, for example by distillation of the Isoprene Concentrate.

4. Piperylene Concentrate

Production of Piperylene Concentrate (cis- and trans-1,3-pentadiene) from Pyrolysis C5s is accomplished by first "heat soaking" the stream in order to dimerize 1,3-cyclopentadiene (CPD). This is necessary because the boiling point of CPD is within 2.5 °F of that of trans-1,3 pentadiene. The heat soak produces a mixture of CPD dimer and codimers (DCPD Concentrate) that can be removed as a bottoms product from the balance of the Pyrolysis C5 stream. After removal of the DCPD Concentrate, what is left of the Pyrolysis C5s can be charged to a distillation column (the isoprene-piperylene splitter) to yield Piperylene Concentrate as a bottoms product. The carbon number distribution for Piperylene concentrate is predominantly C5. A typical Piperylene Concentrate stream composition includes 60% piperylenes, 10% 2-methyl-2-butene, and about 0.2% benzene.

5. Isoprene Concentrate

The isoprene-piperylene splitter described for the above stream also yields Isoprene Concentrate as a distillate. The carbon number distribution for Isoprene concentrate is predominantly C5. A typical Isoprene Concentrate stream contains 40% isoprene with the balance largely iso- and n-pentane and C5 monolefins. Pentenes, as described for the Pentenes stream, may or may not have been removed in the distillation sequence and this has the corresponding effect on the concentration of the lower boiling pentene and pentane components in the Isoprene Concentrate.

6. Isoprene-Piperylene Concentrate

The intermediate process stream charged to the isoprene-piperylene splitter (as described above for piperylene concentrate) is sometimes isolated as a product. This stream typically contains about 20% isoprene and 14% piperylenes.

7. Isoprene, High Purity

High purity isoprene (98+%) is produced by separation from isoprene concentrate. This is accomplished using an extractive distillation process.

8. Isoprene Purification Byproduct

Isoprene Purification Byproduct is a byproduct from the Isoprene purification process.
The carbon number of the stream is predominantly C5 and the composition is largely iso- and n-pentane, plus lesser amounts of pentenes and about 5% isoprene. The byproduct may also contain 1,3-butadiene at about 0.5%.

9. 2-Methyl-2-Butene

The component 2-methyl-2-butene is sometimes separated from a mixed C5 stream by first converting to an intermediate, then separating the intermediate from the mix by distillation, and then cracking the intermediate back to yield product 2-methyl-2-butene.

10. Metathesis Byproduct

An olefins plant may include a Metathesis process which converts ethylene and/or butenes into propylene. This process produces a byproduct (referred to here as Metathesis Byproduct). The stream is a gasoline stream consisting primarily of C5 and C6 olefins.

11. Neohexene

Neohexene is a high purity product (typically 97% 3,3-dimethyl-1-butene), derived by reaction of diisobutylene and ethylene.

III. TEST PLAN RATIONALE

A. Overview

Human Health Effects

In addition to a nearly complete HPV SIDS (Screening Information Data Sets) data set for isoprene and genetic toxicity data for 2-methyl-2-butene, a substantial amount of toxicity data are available for

many of the other components of the streams in the C5 Non-Cyclics category. Some of the components are SIDS materials, and some components will be tested by the American Chemistry Council Olefins Panel within other category test plans or by other groups within the HPV or ICCA programs.

Based on examination of existing data for components of the streams in the C5 Non-Cyclics category, isoprene and, to a lesser extent, 2-methyl-2-butene are expected to be the most biologically active of the major components in the category and thus the major contributors to toxicological activity, with genotoxicity the endpoint of concern. Of the SIDS endpoints, only the genetic toxicity tests are known to show a dose-related adverse response with isoprene. With the exception of acute central nervous system effects at high concentrations, none of the other components that are present in substantial amounts in these streams has demonstrated a potential to cause significant adverse health effects.

It is anticipated that the biological spectrum of activity for isoprene, with regard to positive genetic toxicity, may be reflected in other streams in this category that contain isoprene. However, since metabolism of isoprene is required for toxicity, and other C5 alkenes are metabolized through a common metabolic pathway, it is anticipated that mixed components will compete for the same active enzyme sites. Different individual toxicities, which are dependent on the formation of biologically active metabolites, may be reduced, as less metabolite(s) will be produced through competition for these sites. Hence the positive genotoxicity of isoprene, or the less potent 2-methyl-2-butene, may in fact be reduced or eliminated by the greater presence of the other components. This can only be assessed by testing a mixed stream.

Thus, the strategy for characterizing the hazards of this group is based on testing a representative product with mid-range isoprene content (14-20%) and one with low isoprene content (approximately 2%) in full SIDS human health test batteries (except for acute inhalation toxicity which is not deemed informative for the HPV Challenge Program). The following tests will be conducted: A bacterial gene mutation test (Ames test, OECD Guideline 471), a mouse inhalation micronucleus test for chromosome aberrations (OECD Guideline 474), and a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422). This strategy will allow an evaluation of the impact of isoprene on the toxicity of the mixed streams, and will also allow an assessment of the hazards of the other components when the influence of isoprene is reduced or eliminated. The streams tested will include other chemical components representative of other streams that make up this category. The exact composition of the streams to be tested will be determined analytically at the time of testing. In addition, the SIDS human health data set (except for the acute inhalation toxicity test which is not deemed informative for the HPV Challenge Program) will be completed for 2-methyl-2-butene. The following tests will be conducted: A bacterial gene mutation test (Ames test, OECD Guideline 471), a mouse inhalation micronucleus test for chromosome aberrations (OECD Guideline 474), a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422). 2-Methyl-2-butene is sponsored through the ICCA HPV Program.

The inhalation route of exposure was chosen for the health effects testing because inhalation is the most

relevant route of exposure for the C5 Non-Cyclics streams. The mouse micronucleus test was chosen for chromosomal effects testing because isoprene is negative in *in vitro* tests but positive in the mouse micronucleus test. 2-Methyl-2-butene is also positive in the mouse micronucleus test. The mouse is the standard species for micronucleus tests and a substantial historical database exists for the mouse in this test. The rat will be used in the repeated dose/reproductive and developmental effects/neurotoxicity screen because this test was designed for the rat and there is a historical data base for the rat but not for the mouse. The rat is also the standard species for reproductive toxicity tests. Furthermore, there is a substantial amount of data developed in rats, mice, primates, and humans (*in vitro*) providing strong support for the proposition that the rat is a scientifically more appropriate model for humans than is the mouse.

The recommended testing, together with existing data and data for the components under development by the American Chemistry Council Olefins Panel for other categories under the HPV program, by other HPV consortia, and by the OECD SIDS program, will be sufficient to adequately characterize the toxicity of the range of substances included in this category.

Physical-Chemical Properties

Physicochemical data for each of the 11 streams in the C5 Non-Cyclics category will be developed using the EPIWIN© model[1], as discussed in the EPA document titled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program."

Ecotoxicity

The product streams of this category are expected to cause similar moderate acute aquatic toxicity to freshwater fish and invertebrates and moderate toxicity to freshwater algae. This is based on existing data for similar saturated hydrocarbons and results of computer modeling using ECOSAR for selected chemical components of this category [ECOSAR is an aquatic toxicity modeling program and is a subroutine contained in EPIWIN[1]]. In addition, isoprene and 2-methyl-2-butene, which are contained by several streams in this category, are also expected to exhibit a similar degree of toxicity as the streams. To demonstrate the expected toxic effects in each of three aquatic organisms, the Panel will test the following streams and chemicals:

- Pyrolysis C5s: A product stream with mid-range isoprene content (approximately 14-20%);
- Hydrotreated C5s: A product stream with low isoprene content (approximately 2%);
- 2-methyl-2-butene (sponsored through ICCA HPV Program); and
- isoprene (sponsored through ICCA HPV Program).

The testing for all these materials except isoprene will include an alga toxicity test (OECD Guideline 201), a *Daphnia* sp. acute toxicity test (OECD Guideline 202), and a fish acute toxicity test (OECD Guideline 203). Because isoprene is contained in the two streams, the Panel will also conduct one test, an algal toxicity test, with a high purity isoprene to confirm that the results are similar to the two tested

streams and 2-methyl-2-butene. An alga was selected because it was calculated by ECOSAR to be the more sensitive organism of the three aquatic trophic levels included in the HPV Program. In addition, structural activity relationships will be used to predict toxicity to fish and *Daphnia*.

Environmental Fate

A biodegradation test via manometric respirometry (OECD Guideline 301F) will be conducted on a representative product with mid-range isoprene content (approximately 14-20%), one with low isoprene content (approximately 2%), and 2-methyl-2-butene. This test guideline uses a closed test system, which is required when assessing the biodegradation of volatile materials like those in this category. It is also recommended when evaluating mixtures containing several chemical species, some of which may have minimally water-soluble components.

The endpoints for photodegradation, hydrolysis, transport, and fugacity will be either calculated or discussed. Chemical equilibrium models are used to calculate fugacity, which is only calculated. Chemical components of process streams in the C5 Non-Cyclics category are calculated to partition primarily to the air, and therefore their fate in air is of environmental interest (this is discussed below under photodegradation). In addition, these components have relatively low Kow values, which suggest that they will not tend to partition to suspended organic matter in air and precipitate to aquatic and terrestrial compartments.

1. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline[2]. UV light absorption of the 11 streams in the category will be evaluated to identify those having the potential to degrade in solution. For those compounds with a potential for direct photolysis in water, first order reaction rates will be calculated.

2. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured[3] (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA[4]. An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Light hydrocarbons, such as those in the C5 Non-Cyclics category, readily volatilize to air. In air, chemicals may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows)[1] is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH reaction rate constant, a 12-hr day, and a given OH concentration. This calculation will be performed for the representative components of the 11 streams in the C5 Non-Cyclics category.

3. Stability in Water (Hydrolysis Testing and Modeling)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters[5]. Stability in water can be measured[3] (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA[4]. An estimation method accepted by the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows)[1] is used by OPPTS.

All of the chemical structures included in the C5 Non-Cyclics category are simple hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared describing the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

4. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model[6]. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data*[3], which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for representative chemical components identified in streams in this category. A computer model, EPIWIN – version 3.02[1], will be used to calculate the properties needed to run the Level I EQC model.

B. Stream Specific Rationales

The rationales for the test plan strategy specific to each stream in the C5 Non-Cyclics category are presented below:

1. Pyrolysis C5s

This stream will be tested in a complete SIDS battery of tests (except for acute toxicity) to assess the toxicity of streams with a mid-range (approximately 14-20%) isoprene content in addition to significant amounts of other C5 dienes, 2-methyl-2-butene, dicyclopentadiene, and most of the other C5s that are present in the other streams in the C5 Non-Cyclics Category.

2. Hydrotreated C5s

This stream will be tested in a complete SIDS battery of tests (except for acute toxicity) to assess the toxicity of streams with a low (approximately 2%) isoprene content; small amounts of other C5 dienes; no dicyclopentadiene; substantial concentrations of pentenes, pentanes, cyclopentene; and approximately 11% 2-methyl-2-butene.

3. Pentenes

This stream is similar to the Hydrotreated C5s stream except that it contains approximately 4% 2-methyl-2-butene. The toxicity profile of this stream is expected to be the same as that of the Hydrotreated C5s stream. No testing is proposed for this stream at this time.

4. Piperylene Concentrate

This stream is similar to the Hydrotreated C5 stream except for the presence of 2-methyl-2-butene (typically 5-15%) and a large amount of 1,3-pentadiene (typically 30-60%). The toxicity of the Piperylene Concentrate stream can be characterized by data for 2-methyl-2-butene, 1,3-pentadiene, and the Hydrotreated C5s stream. 1,3-Pentadiene is an OECD SIDS material and all SIDS endpoints have been adequately addressed. The SIDS Initial Assessment Report (SIAR) indicates that 1,3-pentadiene (cis and trans combined) is of low concern for further testing, and proposes no additional testing. Testing of 2-methyl-2-butene and the Hydrotreated C5s stream is proposed in this Test Plan.

5. Isoprene Concentrate

This stream is similar to the Pyrolysis C5s stream except that this stream has a higher concentration of isoprene. Existing data for high purity isoprene and data from testing of the Pyrolysis C5s stream, which has approximately 14-20% isoprene, can be used to characterize the toxicity of Isoprene Concentrate. No additional testing is proposed for this stream at this time.

6. Isoprene-Piperylene Concentrate

This stream is similar to the Pyrolysis C5s stream. Data from testing of the Pyrolysis C5s stream, which has approximately 14-20% isoprene, can be used to characterize the toxicity of Isoprene-Piperylene Concentrate. No additional testing is proposed for this stream at this time.

7. Isoprene, High Purity

Isoprene has been extensively tested and all HPV endpoints except for aquatic toxicity have been adequately addressed. A significant amount of additional toxicology data is also available. An algal toxicity test is proposed for this stream. In addition, structural activity relationships will be used to predict toxicity to fish and Daphnia. Isoprene is sponsored through the ICCA HPV Program.

8. Isoprene Purification Byproduct

This stream is predominantly (50-70%) isopentane, which is being addressed by the American Chemistry Council Hydrocarbon Solvents Panel, but also has a typical isoprene content of 1-12%. The non-genetic endpoints can be addressed by the data for isopentane. The data for isoprene, Pyrolysis C5s and Hydrotreated C5s streams can be used to characterize the genetic toxicity of this stream. No additional testing is proposed for this stream, at this time.

9. 2-Methyl-2-Butene

This stream is typically 93% 2-methyl-2-butene and 6.7% 2-methyl-1-butene. It will be tested in a complete battery of tests except for genetic toxicity tests (which are available). 2-Methyl-2-butene is sold as a high-purity material and is also a component in the Pyrolysis C5s, Hydrotreated C5s, Pentenes, Isoprene Concentrate, Piperylene Concentrate, and Isoprene-Piperylene Concentrate streams. 2-Methyl-2-butene is sponsored through the ICCA HPV Program.

10. Metathesis Byproduct

This stream contains approximately 3% 2-butene, 44% pentenes, and 51% hexenes and is predicted to have a toxicology profile similar to that of the 2% isoprene stream. The toxicity of the Metathesis Byproduct stream can be adequately characterized by read-across from data for 1-hexene, which is an OECD SIDS material, and from a C6-C8 internal olefin (or similar) stream which will be tested by the American Chemistry Council Higher Olefins Panel and from results for the hydrotreated C5s stream, if test results indicate that the presence of 2% isoprene does not cause genetic effects.

11. Neohexene

This stream is typically 97% neohexene (3,3-dimethyl-1-butene) and 3% related hydrocarbons. Based on existing acute and genetic toxicity data, neohexene is expected to have a toxicity profile similar to that

of many of the C5 and C6 alkenes present in the streams in this category. The toxicity of neohexene is also expected to be similar to that of the low isoprene stream, Hydrotreated C5s, for which testing is proposed in this Test Plan. Existing data for neohexene and similar alkenes and the data from the proposed testing of the Hydrotreated C5s stream are expected to be adequate to characterize the toxicity of this stream.

IV. TEST PLAN SUMMARY

The following testing, modeling, and technical discussions will be developed for the C5 Non-Cyclics category (Table 3):

- Conduct one test battery for all SIDS human health endpoints (except acute toxicity) on a stream containing approximately 14-20% isoprene, Pyrolysis C5s (exact composition to be determined at the time of testing). The following studies will be conducted: An Ames test (OECD Guideline 471), a mouse inhalation micronucleus test (OECD Guideline 474), and a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422).

- Conduct one test battery for all SIDS human health endpoints (except acute toxicity) on a stream containing approximately 2% isoprene, Hydrotreated C5s (exact composition to be determined at the time of testing). The following studies will be conducted: An Ames test (OECD Guideline 471), a mouse inhalation micronucleus test (OECD Guideline 474), and a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422).

- Conduct a rat inhalation combined repeated dose/reproductive and developmental effects/neurotoxicity screen (OECD Guideline 422) on a high purity 2-methyl-2-butene stream (exact composition to be determined at the time of testing). 2-Methyl-2-butene is sponsored through the ICCA HPV Program.

- Compare endpoints evaluated for the Pyrolysis C5s stream (the mid-range isoprene stream with approximately 14-20% isoprene) and the Hydrotreated C5s stream (the low isoprene stream with approximately 2% isoprene) to those for high purity isoprene and the other identified data and prepare a technical discussion in terms of their representation of potential human health effects for this category.

- Compare endpoints evaluated for the 2-methyl-2-butene stream to those for the other two tested streams and the other identified data and prepare a technical discussion in terms of their representation of potential human health effects for this category.

- Conduct alga toxicity tests (OECD Guideline 201), *Daphnia* sp acute toxicity tests (OECD Guideline 202) and fish acute toxicity tests (OECD Guideline 203) with a mid-range

isoprene stream (Pyrolysis C5s), low isoprene stream (Hydrotreated C5s), and 2-methyl-2-butene.

- Conduct an alga toxicity study (OECD Guideline 201) with high purity isoprene. Isoprene is sponsored through the ICCA HPV Program. In addition, structural activity relationships will be used to predict toxicity to fish and *Daphnia*.

- Conduct biodegradation tests (OECD Guideline 301F) with mid-range (Pyrolysis C5s) and low isoprene (Hydrotreated C5s) streams and 2-methyl-2-butene.

- Prepare a technical discussion of the potential aquatic toxicity of selected chemical components comprising streams in this category using modeled data.

- Prepare a technical discussion on the potential of chemical components comprising streams in this category to photodegrade.

- Prepare a technical discussion on the potential of chemical components comprising streams in this category to hydrolyze.

- Calculate fugacity data for selected chemical components of streams in this category.

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program*.

Summaries of results will be developed once the data and analyses are available. This test plan is expected to provide adequate data to characterize the human health effects and environmental fate and effects endpoints for the category under the Program.

V. OTHER SUPPORTING DATA

The test plan is based on the expectation that the biological activity of isoprene and 2-methyl-2-butene will be responsible for any effects seen in the testing of the C5 Non-Cyclics streams. This expectation is based on a review of a substantial amount of data that is available for many of the other components of the C5 Non-Cyclics category. Existing data is indicated in Table 4.

Additional data for components of the C5 Non-Cyclics streams that will provide support for this category will be collected by other test plans within the Olefins Panel's HPV program (see Table 5), by other consortia participating in the HPV or ICCA programs, or from chemicals sponsored in the OECD SIDS program:

- 1-Butene: Data gaps will be filled under the Olefins Panel's Low Butadiene C4 HPV Test Plan.

1-Butene is sponsored through the ICCA HPV Program.

- 2-Butene: OECD SIDS
- n-Pentane: Included in American Petroleum Institute's HPV Test Plan.
- C5 Aliphatic Category: Included in the American Chemistry Council Hydrocarbon Consortium HPV Test Plan that covers n-pentane, isopentane, and cyclopentane.
- 1-Pentene and isopentene: Although not covered by the American Chemistry Council Higher Olefins Panel's HPV Test Plan, the data obtained for hexenes within that program can be used for read-across to the pentenes. In addition, data for 1-hexene collected as part of the OECD SIDS program can be used for read-across.
- Cyclopentane: Included in American Chemistry Council Hydrocarbon Solvents Panel's HPV program.
- 1,3-Pentadiene: OECD SIDS
- Dicyclopentadiene: OECD SIDS

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Table 1. CAS Numbers and Descriptions Associated with Streams in C5 Non-Cyclics Category

CAS Number	CAS Number Description
513-35-9	2-Butene, 2-methyl-
558-37-2	1-Butene, 3,3-dimethyl-
64742-83-2	Naphtha, petroleum, light steam-cracked
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68476-43-7	Hydrocarbons, C4-6, C5-rich
68476-55-1	Hydrocarbons, C5-rich
68477-35-0	Distillates, petroleum, C3-6, piperylene-rich
68514-39-6	Naphtha, petroleum, light steam-cracked, isoprene-rich
68527-11-7	Alkenes, C5
68527-19-5	Hydrocarbons, C1-4, debutanizer fraction
68603-00-9	Distillates, petroleum, thermal cracked naphtha and gas oil
68603-03-2	Distillates, petroleum, thermal cracked naphtha and gas oil, extractive
68606-29-1	Hydrocarbons, C4 and C8, butene concentrator by-product
68606-36-0	Hydrocarbons, C5-unsatd. rich, isoprene purifn. by-product
68956-55-8	Hydrocarbons, C5-unsatd.
78-79-5	1,3-Butadiene, 2-methyl-

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition)

Table 2. Typical Stream Compositions (%) for the C5 Non-Cyclics Category

Component	Pyrolysis C5s	Hydrotreated C5s	Pentenes	Piperylene Concentrate	Isoprene Concentrate	Isoprene - Piperylene Concentrate	Isoprene	Isoprene Purification Byproduct	2-Methyl-2-Butene	Metathesis Byproduct	Neohexene
Isoprene (2-Methyl-1,3-Butadiene)	9 - 25	2	2.4	0 - 6	14 - 80	20	99.7	1 - 12			
1,4-Pentadiene	1 - 6		1		0 - 4	3		1 - 10			
1,3-Pentadiene (isomer mix)	6 -23	2		31 - 60	1 - 15	14					
3-Methyl-1,2-Butadiene					3.5						
1,3-Butadiene	0 - 3							0 - 1			
1,2-Butadiene					1.2						
1,3-Cyclopentadiene	2 - 23	5		1 - 4	0 - 15	2		0 - 1			
Dicyclopentadiene	1 - 19			0 - 1	0.4						
Cyclopentene	1 - 11	15 - 20		8 - 20	0 - 10	4					
Cyclopentane	0 - 2	2		1 - 5	8 - 15	1					
Isopentene		15 - 20									
1-Pentene (Amylene)	3 - 12		13.7		0 - 10	6		3 - 11		3	
2-Pentene (isomer mix)	2 - 10		18	1 - 10	1 - 16	5		3 - 9		41	
2-Methyl-2-Butene	1 - 5	11	4	5 - 15	0 - 9	3			93		
2-Methyl-1-Butene	1 - 8		17.5		1 - 16	6			6.7		
3-Methyl-1-Butene (Isoamylene)	0 -12				0 - 1	1					
Methyl Butenes								3 - 21			
Isopentane (2-Methylbutane)	3 - 29	15 - 25	12.3		21	16		50 - 70			
n-Pentene		10 - 15									
Pentane	4 - 30	15 - 20	31.7	0 - 5	0 - 26	16		0 - 10			
3-Methyl- 1,4-Pentadiene				1.7							
3-Methyl-1-Pentene	0 - 2										

Component	Pyrolysis C5s	Hydrotreated C5s	Pentenes	Piperylene Concentrate	Isoprene Concentrate	Isoprene - Piperylene Concentrate	Isoprene	Isoprene Purification Byproduct	2-Methyl-2-Butene	Metathesis Byproduct	Neohexene
Methylpentenes				5							
2,3-Dimethy-1-Butene											1.5
C6 Hydrocarbons	2 - 4		1	1 - 5	0 - 3						
1-Hexene	0 - 3									4	
2-Hexene										15	
3-Hexene										8	
Hexenes		1		2							
Methyl-2-Pentenes										24	
2,2-Dimethylbutane (neohexane)	0 - 1			2.7							
3,3-Dimethyl-1-Butene (Neohexene)											97
2-Methylpentane		5									
Methylpentanes				16							
Hexane		1		3.3							
Benzene	0 - 1	1		0.2							
Dimers of CPD with other C4 and C5 Dienes, excluding DCPD	0 - 2										
2-Butyne (Dimethylacetylene)	0 - 2				1 - 2						
1-Butene		2									
2-Butene (isomer mix)	0 - 1				1 - 20					3	

same Note 1:The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 2: The listed ranges should not be considered absolute values. They are instead the approximate highs and lows of the reported values, and are expected to be typical limit values.
Note 3: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the stream

(composition).

Table 3. Assessment Plan for C5 Non-Cyclics Category Under the Program. Robust summaries for existing studies are submitted separately.

Stream Description	Human Health Effects						Ecotoxicity			Environmental Fate				
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
C5 Non-Cyclics Streams Containing Isoprene														
Isoprene (1,3-Butadiene, 3-methyl) , High Purity (Isoprene Content = 100%) *	Ö	Ö	Ö	Ö	Ö	Ö	CM	CM	T	CM	CM/TD	TD	CM	Ö
Isoprene Concentrate (Isoprene Content = 14-85%)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C5s (Isoprene Content = 14-20%)	NA	T	T	T	T	T	T	T	T	CM	CM/TD	TD	CM	T
Isoprene-Piperylene Concentrate (Isoprene Content = 20%)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Isoprene Purification Byproduct (Isoprene Content = 1-12%)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Piperylene Concentrate (Isoprene Content = 0-6%)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pentenes (Isoprene Content = 2%)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C5s (Isoprene Content = 2%)	NA	T	T	T	T	T	T	T	T	CM	CM/TD	TD	CM	T
Streams Not Containing Isoprene but Containing Other Components Found in Streams in C5 Non-Cyclics Category														
2-Methyl-2-Butene (≥ 93%)*	NA	Ö	Ö	T	T	T	T	T	T	CM	CM/TD	TD	CM	T
Metathesis Byproduct (Pentenes, Hexenes)	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Neohexene (3,3-dimethyl-1-Butene, ≥97%)	Ö	Ö	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA

Ö Adequate existing data available TD Technical discussion proposed RA Read Across (see Sec. III.B)
CM Computer Modeling proposed T Proposed Testing * Sponsored through ICCA

NA Not Applicable

Table 4. Existing Data for Components Other Than Isoprene and 2-Methyl-2-Butene

(Robust summaries for these studies will not be submitted with the Test Plan; some studies have not been reviewed for adequacy)

		Human Health Effects						Ecotoxicity			Environmental Fate				
CAS Number	**Chemical Name**	**Acute Oral**	**Genetic Point Mutation**	**Genetic Chrom. Aberr.**	**Sub-chronic**	**Develop-mental**	**Repro-duction**	**Acute Fish**	**Acute Invert.**	**Algal Toxicity**	**Physical Chem.**	**Photo-degra-dation**	**Hydro-lysis**	**Fugacity**	**Biodegra-dation**
78-78-4	Isopentane (2-methyl-butane)	√	√		√										√
590-18-1	Cis-2-butene	√													
109-66-0	Pentane	√	√	√	√	√		√	√	√					√
107-83-5	2-Methylpentane (isohexane)				√										
646-04-8	Trans-2-pentene				√										
142-29-0	Cyclopentene	√													
287-92-3	Cyclopentane	√			√										
504-60-9	1,3-Pentadiene (SIDS SIAR complete)	√	√	√	√	√	√	√	√	√					√
542-92-7	Cyclopentadiene	√			√										
26760-64-5	2-methyl-1-butene			√											
77-73-6	Dicyclopentadiene	√	√	√	√	√	√	√	√	√					√
110-54-3	Hexane	√	√	√	√	√	√	√	√						

Table 5. American Chemistry Council Olefins Panel Sponsored HPV Test Categories

Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7	Resin Oil - High Dicyclopentadiene
8	Resin Oil - Low Dicyclopentadiene
9	Cyclodiene Concentrates
10	Fuel Oils

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers".

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two

or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. It is a subset of these mixed streams that make up the constituents of the C5 Non-Cyclics category.

The chemical process operations that are associated with the process streams in the C5 Noncyclics category are shown in Figure 1.

Figure 1. Chemical process operations associated with process streams in the C5 Noncyclics category.